

More on volume dependence of spectral weight functions*

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Spectral weight functions are easily obtained from two-point correlation functions and they might be used to distinguish single-particle from multi-particle states in a finite-volume lattice calculation, a problem crucial for many lattice QCD simulations. In previous studies, it is shown that the spectral weight function for a broad resonance shares the typical volume dependence of a two-particle scattering state i.e. proportional to $1/L^3$ in a large cubic box of size L while the narrow resonance case requires further investigation. In this paper, a generalized formula is found for the spectral weight function which incorporates both narrow and broad resonance cases. Within Lüscher's formalism, it is shown that the volume dependence of the spectral weight function exhibits a single-particle behavior for a extremely narrow resonance and a two-particle behavior for a broad resonance. The corresponding formulas for both A_1^+ and T_1^- channels are derived. The potential application of these formulas in the extraction of resonance parameters are also discussed.

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I. INTRODUCTION

Lattice Chromodynamics (lattice QCD) has provided us with a genuine non-perturbative theoretical framework to study low-energy physics in strong interactions from first principles. Combined with numerical Monte Carlo simulations, lattice QCD has become a crucial player in hadron spectroscopy and other studies in the field.

In a typical lattice simulation, one computes a two-point function of an appropriate operator with a definite quantum number via Monte Carlo simulation and the energy eigenvalues in that sector are then extracted from the time-dependence of the correlation function. In fact, the correlation function of an operator \mathcal{O} may be written schematically as: $C(t) = \langle \mathcal{O}(t)\mathcal{O}(0) \rangle = \sum_n W_n(E_n) e^{-E_n t}$ where E_n 's are the energy eigenvalues of the QCD Hamiltonian for the corresponding state n with the quantum numbers associated with the operator \mathcal{O} . The functions $W_n(E_n)$ are the so-called spectral weight functions for the state n . Since lattice simulations are all performed in a finite volume, the eigenvalues E_n are all discrete in nature. This poses a question on the particle nature of the corresponding state. If in the infinite volume, single-particle and multi-particle states are different in the sense that the spectra for single particle states are discrete while that for multi-particle states are continuous starting from the multi-particle threshold. In a finite volume, however, it is not an easy task to tell whether a state with a particular energy E_n is a

single- or a multi-particle state since all states have become discrete. This distinction is not only for academic purposes but also of phenomenological importance as well if one recalls that quite a number of new resonance-like structures have been identified rather close to the multi-particle threshold of known hadrons. To cope with this problem, it has been suggested that the volume dependence of the spectral weight functions $W_n(E_n, L)$, which is also a function of the box size L , may be used as a probe to distinguish single- and multi-particle states [1]. With an appropriate normalization, it is argued that the spectral weight function for a single-particle state has little volume dependence while that for a two-particle state will exhibit a $1/L^3$ behavior.

In our previous study [2], it was shown that the above mentioned criteria becomes invalid for a broad resonance. Instead of showing little volume dependence, the spectral weight function for a broad resonance will exhibit a $1/L^3$ behavior, typical for two-particle states. However, our previous study does not apply for extremely narrow resonances. In this paper, we re-examine the problem within Lüscher's formalism (see Ref. [3]), with an emphasis on the narrow resonance limit case. A generalized formula is found which incorporates both narrow and broad resonance cases. The conclusion we reached is exactly analogous to what we discovered in a model study [4], namely that for a broad resonance, the spectral weight behaves like a multi-particle state while for an extremely narrow resonance, a single-particle behavior realizes. We also point out the possibility to extract the resonance parameters from the spectral weight function. We closely follow the discussion of our previous work [2]. The reader is referred to that reference for notations and further details.

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II. THE MODEL IN THE INFINITE VOLUME AND THE SIGNATURE OF A RESONANCE

In the infinite volume, consider a non-relativistic quantum mechanical model with Hamiltonian given by:

$$H = -\frac{1}{2m}\nabla^2 + V(r) , \quad (1)$$

where the potential $V(\mathbf{r})$ is zero for $r > a$ with some $a > 0$. We now discuss the energy eigenstates satisfying: $H\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$. One can expand the eigenfunction as: $\Psi(\mathbf{r}) = \psi_{lm}(r)Y_{lm}(\mathbf{n})$ with: $\mathbf{r} = r\mathbf{n}$ and $\psi_{lm}(r)$ is the radial wave-function satisfying the radial Schrödinger equation:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 - 2mV(r) \right) \psi_{lm}(r) = 0 . \quad (2)$$

where $E = k^2/(2m)$ being the energy eigenvalue of the state. There exists a unique solution to the radial Schrödinger equation that is bounded near the origin which is denoted as: $u_l(r; k)$ and the general solution to the radial Schrödinger equation has the form: $\psi_{lm}(r) = b_{lm}u_l(r; k)$ with some constant b_{lm} to be fixed by other conditions.

In the region $r > a$ where the interaction vanishes, the solution $u_l(r; k)$ are expanded in terms of spherical Bessel functions: [7]

$$u_l(r; k) = \alpha_l(k)j_l(kr) + \beta_l(k)n_l(kr) . \quad (3)$$

The coefficients $\alpha_l(k)$ and $\beta_l(k)$ have simple relation with the scattering phase shift:

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)} , \quad \cot \delta_l(k) = \frac{\alpha_l(k)}{\beta_l(k)} . \quad (4)$$

In the low-energy limit $k \rightarrow 0$, one normally defines:

$$\alpha_l^0 = \lim_{k \rightarrow 0} k^l \alpha_l(k) , \quad \beta_l^0 = \lim_{k \rightarrow 0} k^{-l-1} \beta_l(k) , \quad (5)$$

and the threshold parameters $a_l \equiv \beta_l^0/\alpha_l^0$. In particular, a_0 for $l = 0$ is referred to as the s -wave scattering length. The threshold parameters a_l are important because they characterize most behaviors in low-energy scattering processes. For example, we have:

$$\delta_l(k) \simeq a_l k^{2l+1} + O(k^{2l+3}) , \quad (\text{mod } \pi) . \quad (6)$$

To fix the normalization of $u_l(r; k)$, we impose the condition: [8]

$$u_l(r; k) \simeq \frac{1}{kr} \sin(kr - l\pi/2 + \delta_l) . \quad (7)$$

Another way of writing the asymptotic behavior of the radial wave function in Eq. (3) is as follows:

$$u_l(r; k) \simeq \frac{1}{r} [A_l(k)e^{ikr} + B_l(k)e^{-ikr}] , \quad (8)$$

where the functions $A_l(k)$ and $B_l(k)$ are related to the coefficients $\alpha_l(k)$ and $\beta_l(k)$ via

$$A_l(k) = (-i)^l(\beta_l - i\alpha_l)/(2k), B_l(k) = (+i)^l(\beta_l + i\alpha_l)/(2k). \quad (9)$$

When regarded as functions of the energy $E = k^2/(2m)$, we will write them as $A_l(E)$ and $B_l(E)$, respectively. Note that for real positive energy, we have:

$$A_l(E) = B_l(E)^* , \quad E > 0, E \in \mathbb{R} . \quad (10)$$

The condition for a narrow resonance is that, the coefficient $B_l(E)$ has a complex zero on the second Riemann sheet at $E = E_\star - i\Gamma/2$, close to the real axis:

$$B_l\left(E_\star - i\frac{\Gamma}{2}\right) = 0 , \quad (11)$$

with Γ being the physical width of the resonance. In this case, the scattering properties of the system is mainly governed by the position of this resonance pole, if the scattering energy E is very close to the resonance energy E_\star . In fact, since the function $B_l(E)$ vanishes at $E_\star - i\Gamma/2$, for real energy E close to E_\star , we may approximate the function by:

$$B_l(E) \simeq b_l(E - E_\star + i\Gamma/2) , \quad (12)$$

for some complex constant b_l . Therefore, for positive real energy E close to E_\star , the radial wavefunction looks like

$$u_l(r; k) \simeq \frac{1}{r} [b_l^*(E - E_\star - i\Gamma/2)e^{ikr} + h.c.] . \quad (13)$$

This then shows that the phase-shift near the resonance point is given by

$$e^{2i\delta_l(E)} = e^{2i\delta_l^{(*)}} \left(\frac{E - E_\star - i\Gamma/2}{E - E_\star + i\Gamma/2} \right) , \quad (14)$$

where the quantity $\delta_l^{(*)}$ is given by

$$e^{2i\delta_l^{(*)}} = (-1)^{l+1} (b_l^*/b_l) . \quad (15)$$

This is a constant phase (meaning that it does not depend on the energy substantially in the resonance region) which depends only on the position of the resonance. The energy dependent part of the phase shift is given solely by the factor in the big parenthesis in Eq. (14). It is seen that, for extremely narrow resonance, the phase shift jumps by π when the energy passes through E_\star within an energy range of order of several Γ .

Another important point has become clear from the expansion in Eq. (13). If we set the energy E to be exactly the resonance energy E_\star , the expression u_l is vanishing if Γ becomes infinitesimally small. This means that, to properly normalize the wave-function, therefore, the coefficients b_l has to be of order $1/\Gamma$.

III. THE MODEL ON A TORUS

Now we enclose the system we discussed in the previous section in a large cubic box of size L and impose the periodic boundary condition in all three spatial directions. The potential itself is also periodically continued to $V_L(\mathbf{r}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(|\mathbf{r} + \mathbf{n}L|)$. We define the so-called “outer region” as

$$\Omega = \{\mathbf{r} : |\mathbf{r} + \mathbf{n}L| > a, \text{ for all } \mathbf{n} \in \mathbb{Z}^3\}. \quad (16)$$

This is the region where the potential vanishes identically. We assume $L \gg 2a$ so that the outer region admits free spherical wave solutions (asymptotic states). Following the discussion in our previous paper, we may write the true eigenfunction as:

$$\Psi(\mathbf{r}; k) = \sum_{lm} b_{lm} u_l(r; k) Y_{lm}(\mathbf{n}). \quad (17)$$

where the coefficients b_{lm} are to be determined by boundary conditions and normalization.

In the outer region, the eigenfunctions can also be expanded in terms of singular periodic solutions (SPS) of Helmholtz equation. These are defined as

$$G_{lm}(\mathbf{r}; k) \equiv \mathcal{Y}_{lm}(\nabla) G(\mathbf{r}; k), \quad G(\mathbf{r}; k) = \frac{1}{L^3} \sum_{\mathbf{p}} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}^2 - k^2}. \quad (18)$$

with $\mathcal{Y}_{lm}(\mathbf{r}) \equiv r^l Y_{lm}(\Omega_{\mathbf{r}})$ being the harmonic polynomials. We may write

$$\Psi(\mathbf{r}; k)|_{\mathbf{r} \in \Omega} = \sum_{lm} v_{lm} G_{lm}(\mathbf{r}; k^2). \quad (19)$$

with $|b_4| \ll |b_0|$ in the large volume limit. In the outer region where the interaction vanishes, using relation (3)

In the meantime, the outer solution can also be expanded in terms of spherical harmonics and the spherical Bessel functions $j_l(kr)$, $n_l(kr)$ and the matrix elements $\mathcal{M}_{l'm';lm}(k_i^2)$. The explicit expressions can be found in Ref. [3].

It is also convenient to introduce the cubic version for the functions G_{lm} defined by Eq. (18):

$$\mathcal{G}_{l;i}^{(\Gamma)}(\mathbf{r}; k) = \mathcal{Y}_{l;i}^{(\Gamma)}(\nabla) G(\mathbf{r}; k), \quad (20)$$

where $\mathcal{Y}_{l;i}^{(\Gamma)}(\mathbf{r})$ is the cubic harmonics for a particular representation Γ of the cubic group. The explicit expressions are listed in Appendix A at the end of this paper.

A. Lüscher's formula in A_1^+ and T_1^- channels

In this subsection, we will derive Lüscher's formula in the A_1^+ and T_1^- channel (corresponding to s -wave and p -wave in the continuum, respectively). Using similar arguments and the cubic harmonics given in the appendix, it is easy to generalize the results to other channels.

We first examine the A_1^+ sector which is the analogue of s -wave scattering. A good approximation for the s -wave dominated eigenfunction can be written as a superposition of $l = 0$ and $l = 4$ cubic harmonics with the s -wave component much larger than that of g -wave. So, we may write the eigen-function in A_1^+ sector as:

$$\Psi^{(A_1^+)}(\mathbf{r}; k) = b_0 u_0(r; k) Y_0^{(A_1^+)}(\Omega_{\mathbf{r}}) + b_4 u_4(r; k) Y_4^{(A_1^+)}(\Omega_{\mathbf{r}}) + \dots, \quad (21)$$

we have

$$\Psi^{(A_1^+)}(\mathbf{r}; k)|_{\mathbf{r} \in \Omega} = b_0 [\alpha_0 j_0(kr) + \beta_0 n_0(kr)] Y_0^{(A_1^+)}(\Omega_{\mathbf{r}}) + b_4 [\alpha_4 j_4(kr) + \beta_4 n_4(kr)] Y_4^{(A_1^+)}(\Omega_{\mathbf{r}}) + \dots. \quad (22)$$

On the other hand, in the outer region Ω , we may also expand the wavefunction in terms of cubic SPS of

Helmholtz equation defined in Eq. (20):

$$\Psi^{(A_1^+)}(\mathbf{r}; k)|_{\mathbf{r} \in \Omega} = \left(\frac{4\pi}{k} \right) v_0 \left[\mathcal{G}_0^{(A_1^+)}(\mathbf{r}; k) + \frac{v_4}{k^4} \mathcal{G}_4^{(A_1^+)}(\mathbf{r}; k) + \dots \right]. \quad (23)$$

Matching the above two expansions in the outer region and using the explicit expressions for the cubic harmonics, one arrives at the following result (i.e. Lüscher's formula) for the A_1^+ sector:

$$(\cot \delta^{(0)} - m_{00})(\cot \delta^{(4)} - m_{44}) = m_{40}m_{04} . \quad (24)$$

$$\Psi_3^{(T_1^-)}(\mathbf{r}; k) = b_1 u_1(r; k) Y_{1;3}^{(T_1^-)}(\Omega_{\mathbf{r}}) + b_3 u_3(r; k) Y_{3;3}^{(T_1^-)}(\Omega_{\mathbf{r}}) + \dots , \quad (25)$$

where we have only written out the third component of the vector wavefunction. We may also expand in terms

$$\Psi_3^{(T_1^-)}(\mathbf{r}; k)|_{r \in \Omega} = \left(\frac{4\pi}{k^2} \right) v_1 \left[\mathcal{G}_{1;3}^{(T_1^-)}(\mathbf{r}; k) + \frac{v_3}{k^2} \mathcal{G}_{3;3}^{(T_1^-)}(\mathbf{r}; k) + \dots \right] . \quad (26)$$

Using the explicit expressions for the cubic harmonics and cubic SPS to match the above two equations we obtain Lüscher's formula in the T_1^- sector:

$$(\cot \delta^{(1)} - m_{11})(\cot \delta^{(3)} - m_{33}) = m_{13}m_{31} . \quad (27)$$

Since numerically we have: $m_{11} = m_{00}$, therefore if higher momentum contaminations (i.e. $l \geq 4$ for A_1^+ and $l \geq 3$ for T_1^-) are neglected, the formula in the T_1^- channel has the same form as the one for A_1 channel.

B. Spectral weight function in A_1^+ sector

As we pointed out in our previous study [2], the spectral weight function has to be normalized in a proper manner so that the single-particle states has a conventional behavior. For an interpolating operator $\mathcal{O}(t)$, the state $\mathcal{O}^\dagger(0)|0\rangle$ will generally be a superposition of a tower of energy eigenstates: $\{|E\rangle\}$ with energy eigenvalue E . The spectral weight for a particular energy state $|E\rangle$ obtained from the two-point correlation function of $\mathcal{O}(t)$ is given by:

$$W(E) = |O(E)|^2 = |\langle E | \mathcal{O}^\dagger(0) | 0 \rangle|^2 , \quad (28)$$

where $O(E) = \langle E | \mathcal{O}^\dagger(0) | 0 \rangle$ is the overlap of the exact energy eigenstate $|E\rangle$ with the state $|\mathcal{O}^\dagger(0)|0\rangle$.

The exact energy eigenfunction $\langle \mathbf{r}_1, \mathbf{r}_2 | E \rangle$ only depends on the relative coordinate $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and does not depend on the center-of-mass of the two particles. Therefore, in terms of the wavefunctions associated with the relative

For the sector T_1^- , which is the cubic analogue of the vector channel, we have a similar expression:

of cubic SPS of Helmholtz equation:

motion, the normalization conditions for the A_1^+ and T_1^- channels become:

$$\int_{\mathcal{T}_3} d^3\mathbf{r} |\Psi^{(A_1^+)}(\mathbf{r}; k)|^2 = \frac{1}{L^3} . \quad (29)$$

$$\int_{\mathcal{T}_3} d^3\mathbf{r} \left[\Psi_i^{(T_1^-)}(\mathbf{r}; k) \right]^* \cdot \Psi_j^{(T_1^-)}(\mathbf{r}; k) = \frac{1}{L^3} \delta_{ij} , \quad (30)$$

where $\Psi^{(A_1^+)}(\mathbf{r}; k)$ and $\Psi_j^{(T_1^-)}(\mathbf{r}; k)$ is the wavefunction for the A_1^+ and T_1^- channel respectively.

Let us first investigate the normalization condition in the A_1^+ channel. The integral over the torus in Eq. (29) runs over two regions: the inner region $B = \{\mathbf{r} : r \leq a, \text{ mod } L\}$ where the potential is present and the outer region Ω where it vanishes:

$$\int_B d^3\mathbf{r} |\Psi^{(A_1^+)}(\mathbf{r}; k)|^2 + \int_\Omega d^3\mathbf{r} |\Psi^{(A_1^+)}(\mathbf{r}; k)|^2 = \frac{1}{L^3} . \quad (31)$$

If we assume that the wavefunction in this sector is dominated by the s -wave component such that

$$\begin{aligned} \Psi^{(A_1^+)}(\mathbf{r}; k)|_{\mathbf{r} \in B} &\simeq b_0 u_0(r; k) Y_{00}(\mathbf{n}) , \\ \Psi^{(A_1^+)}(\mathbf{r}; k)|_{\mathbf{r} \in \Omega} &\simeq \left(\frac{4\pi}{k} \right) v_0 G_{00}(\mathbf{r}; k) , \end{aligned} \quad (32)$$

Matching the above two wavefunctions at $r = a$ will fix the ratio b_0/v_0 . Therefore, we may write: $|b_0|^2 = \zeta |v_0|^2$ with ζ being some positive constant with the dimension of k^{-2} . Therefore, we may express the normalization condition as

$$|v_0|^2 \left[\zeta \int_0^a r^2 |u_0(r; k)|^2 dr + \left(\frac{4\pi}{k} \right)^2 \int_{\Omega} d^3 \mathbf{r} |G_{00}(\mathbf{r}; k)|^2 \right] = \frac{1}{L^3}. \quad (33)$$

If we drop the first term in the bracket in the above equation and approximate the second integral by an integral over the whole torus, we obtain exactly the same formula as we derived in our previous study (see Eq. (38) in Ref. [2] and the discussions about it). Normally, if there were no sharp resonance in the scattering, neglecting of the first term is justified since the second term is proportional L^3 , much larger than any normal term in the large volume limit. However, when an extremely narrow resonance is present, this is *not* the case, as we remarked at the end of Sec. II.

The first term in the normalization condition involves the exact radial wavefunction in the interaction region which seems to depend on the details of the potential. However, although generally speaking we do not know the exact form of the inner wavefunction $u_0(r; k)$, the integral $\int_0^a r^2 |u_0(r; k)|^2 dr$ can be related to the corresponding phase shift via an exact formula: [9]

$$\int_0^a r^2 |u_0(r; k)|^2 dr = 2 \left(a + \frac{d\delta_0(k)}{dk} \right) - \frac{1}{k} \sin 2(ka + \delta_0). \quad (34)$$

Now, if there exists an extremely narrow resonance at a particular energy $E_* = k_*^2/(2m)$, then close to the resonance we have $\cot \delta_0 \simeq -(E - E_*)/(\Gamma/2)$. This implies that:

$$\frac{d\delta_0(k)}{dk} = \frac{k}{m} \frac{d\delta_0}{dE} \simeq \frac{\Gamma/2}{(E_* - E)^2 + \Gamma^2/4}. \quad (35)$$

It is seen that, close to the resonance energy, the derivative $d\delta_0/dk$ is proportional to $1/\Gamma$ in the narrow resonance limit (i.e. when $E \simeq E_*$ and $\Gamma \rightarrow 0$). Therefore, in the narrow resonance limit, such a contribution can become comparable or even larger than the second term that is proportional to L^3 in a finite volume. All the other terms in the integral $\int_0^a r^2 |u_0(r; k)|^2 dr$ are bounded in both the narrow resonance and the large volume limit. Therefore, taking into account of this possibility, the normalization condition for the wavefunction is written as

$$|v_0|^2 \left[\xi + \frac{\zeta \Gamma}{(E_* - E)^2 + \Gamma^2/4} + \left(\frac{4\pi}{k} \right)^2 \int_{\mathcal{T}_3} d^3 \mathbf{r} |G_{00}(\mathbf{r}; k)|^2 \right] = \frac{1}{L^3}, \quad (36)$$

where ξ and $\zeta > 0$ are two constants that are regular in both the large volume and the narrow resonance limit.

The integral in Eq. (36) has been computed in our previous paper with the result [2]:

$$\left(\frac{4\pi}{k} \right)^2 \int_{\mathcal{T}_3} d^3 \mathbf{r} |G_{00}(\mathbf{r}; k)|^2 = \frac{4\pi}{k^2} F'(k^2), \quad (37)$$

with the function $F(k^2)$ defined by

$$F(k^2) \equiv \frac{1}{L^3} \sum_{\mathbf{p}} \frac{f(\mathbf{p}^2)}{\mathbf{p}^2 - k^2}. \quad (38)$$

In the large volume limit, the derivative of this function has the approximate form

$$F'(k^2) \simeq \frac{1}{8\pi k} \cot \delta_0(k) + \frac{k}{4\Delta \mathbf{p}^2} \csc^2 \delta_0(k). \quad (39)$$

Collecting everything together, we obtain the following normalization condition in the A_1^+ sector:

$$|v_0|^2 \left[\xi + \frac{\zeta \Gamma}{(E_* - E)^2 + \Gamma^2/4} + \frac{1}{2k^3} \cot \delta_0(k) + \frac{\pi}{k\Delta \mathbf{p}^2} \csc^2 \delta_0(k) \right] = \frac{1}{L^3}. \quad (40)$$

As discussed above, the second term in the bracket in the

above formula is singular in the narrow resonance limit

($O(1/\Gamma)$) while the fourth term is singular in the large volume limit ($O(L^3)$). All other terms are regular in both limits.

Following similar steps as in our previous paper [2], the spectral weight function in the A_1^+ channel now takes the following form:

$$W^{(A_1^+)}(E) = \frac{4\pi|\varphi_L(k^2)|^2/k^2}{\xi + \frac{\zeta\Gamma}{(E_* - E)^2 + \Gamma^2/4} + \frac{1}{2k^3} \cot \delta_0(k) + \frac{\pi}{k\Delta\mathbf{p}^2} \csc^2 \delta_0(k)} , \quad (41)$$

where the function $\varphi_L(k^2)$ has been introduced in Ref. [2] which has little volume dependence. The main difference between this formula and the one obtained in our previous paper is the appearance of the term $(\zeta\Gamma)/[(E_* - E)^2 + \Gamma^2/4]$ in the denominator. This term becomes singular in the narrow resonance limit (proportional to $1/\Gamma$, as $E = E_*$). If the resonance is not extremely narrow, this term is non-singular and can be absorbed into the constant term ξ and we recover our old result: the resonance acquires a spectral weight function proportional to $1/L^3$, typical for two-particle states. However, if the resonance is extremely narrow such that:

$$\zeta/\Gamma \gg \frac{1}{k\Delta\mathbf{p}^2} , \quad (42)$$

the denominator is dominated by the term containing Γ and the whole spectral weight function has little volume dependence, typical for a single-particle state. It is

also noted that, in this limit, the spectral weight function is proportional to Γ , the physical width of the resonance. This is expected since when the resonance becomes extremely narrow, the coupling of the resonance with the two-particle final states also becomes infinitesimally small (and is proportional to the width as it should). To summarize, Eq. (41) is a generalization of our previous formula in the sense that it incorporates both the large volume and the narrow resonance limit.

C. Spectral weight function in T_1^- sector

Following a similar treatment as in the A_1^+ channel, we can obtain the relevant formulas in T_1^- channel. We construct the state using an interpolating operator of the form:

$$|\Phi\rangle = \mathcal{O}^\dagger(0)|0\rangle = \frac{1}{\sqrt{L^3}} \sum_{\mathbf{P}} \tilde{\Phi}(\mathbf{P}) P_z \left[\tilde{\pi}_1^\dagger(\mathbf{P}, 0) \tilde{\pi}_2^\dagger(-\mathbf{P}, 0) - \tilde{\pi}_2^\dagger(\mathbf{P}, 0) \tilde{\pi}_1^\dagger(-\mathbf{P}, 0) \right] |0\rangle , \quad (43)$$

where we have only taken one component (the third component) of the wavefunctions for a vector state. After factorizing out the center of mass motion, the normalization condition expressed in terms of the wavefunction for the relative motion becomes

$$\int_B d^3\mathbf{r} |\Psi_3^{(T_1^-)}(\mathbf{r}; k)|^2 + \int_\Omega d^3\mathbf{r} |\Psi_3^{(T_1^-)}(\mathbf{r}; k)|^2 = \frac{1}{L^3} , \quad (44)$$

where the first integral is over the interaction region while the second is over the outer region where interaction vanishes identically. For the p -wave dominant wavefunction, we have $\Psi_3^{(T_1^-)}(\mathbf{r}; k)|_{\mathbf{r} \in B} \simeq b_1 u_1(r; k) Y_{10}(\Omega_{\mathbf{r}})$ for the wavefunction in the interaction region and $\Psi_3^{(T_1^-)}(\mathbf{r}; k)|_{\mathbf{r} \in \Omega} \simeq (4\pi/k^2) v_1 G_{10}(\mathbf{r}; k)$ in the outer re-

gion. [10] Matching the two wavefunction at the boundary yields the relation $|b_1|^2 = \zeta' |v_1|^2$ for some positive real constant $\zeta' > 0$. The first integral in Eq. (44) can again be estimated in the same manner as that for A_1^+ sector:

$$\int_0^a r^2 |u_1(r; k)|^2 dr = 2 \left(a + \frac{d\delta_1(k)}{dk} \right) - \frac{1}{k} \sin 2(ka + \delta_1) . \quad (45)$$

Assuming that there exists a resonance at $E = E_*$ in this channel and for energies that are close to this resonance we have: $\cot \delta(E) \simeq -(E - E_*)/(\Gamma/2)$. Following similar derivations, we arrive at the following normalization condition for an energy eigenstate whose energy is in the resonance region:

$$|v_1|^2 \left[\xi' + \frac{\zeta'\Gamma}{(E_\star - E)^2 + \Gamma^2/4} + \frac{3}{2k^3} \cot \delta_1(k) + \frac{\pi}{k\Delta\mathbf{p}^2} \csc^2 \delta_1(k) \right] = \frac{1}{L^3}, \quad (46)$$

where ξ' is some real parameter which is regular in both the narrow resonance and large volume limit. With this

normalization condition in the T_1^- sector, the spectral weight function takes the following form:

$$W^{(T_1^-)}(E) = \frac{16\pi|\alpha + k^2\varphi_L(k^2)|^2/(3k^4)}{\xi' + \frac{\zeta'\Gamma}{(E_\star - E)^2 + \Gamma^2/4} + \frac{3}{2k^3} \cot \delta_1(k) + \frac{\pi}{k\Delta\mathbf{p}^2} \csc^2 \delta_1(k)}, \quad (47)$$

where the constant α is defined by:

$$\alpha \equiv \frac{1}{L^3} \sum_{\mathbf{P}} \tilde{\Phi}(\mathbf{P}) \simeq \frac{1}{(2\pi)^3} \int d^3\mathbf{P} \tilde{\Phi}(\mathbf{P}), \quad (48)$$

Inspecting Eq. (47) we find that, the behavior in the T_1^- sector is the same as in the A_1^+ sector qualitatively. The second term in the denominator is singular in the narrow resonance limit while the fourth term is singular in the large volume limit. Which of these two terms dominates the spectral weight function depends on the size of the following two quantities in the denominator: ζ'/Γ and $1/(k\Delta\mathbf{p}^2)$. For an extremely narrow resonance: $\zeta'/\Gamma \gg 1/(k\Delta\mathbf{p}^2)$ and the spectral weight function is almost volume independent, a typical behavior for a single particle state. On the other hand, if we have $\zeta'/\Gamma \ll 1/(k\Delta\mathbf{p}^2)$ the spectral weight exhibits a $1/L^3$ behavior, typical for a two-particle state.

IV. CONCLUSIONS

In this paper, the volume dependence of the spectral weight function is analyzed with the emphasis on the possible narrow resonances. Generalizing our previous results on this subject, we obtain a formula which incorporates both the large volume limit and the narrow resonance limit. This is summarized in Eq. (41) for the A_1^+ channel and in Eq. (47) for the T_1^- channel. If so desired, formulas for other channels can also be derived similarly using the cubic functions listed in the Appendix. These formulae for the spectral weight functions exhibit the following general feature: near a resonance the spectral weight shows single-particle or multi-particle behavior depending on whether the resonance is narrow or broad in the corresponding box. This is controlled by the size of the two quantities ζ'/Γ and $1/(k\Delta\mathbf{p}^2)$ that appear in the spectral weight function. If the former one dominates, a single particle feature (an almost volume independent spectral weight function) realizes; if the latter one dominates, a two-particle feature emerges with a

$1/L^3$ dependence on the volume for the spectral weight function. Therefore, using the general Lüscher's formalism, we have shown this general feature for the spectral weight function, just as we discovered it in a solvable model in Ref. [4].

Furthermore, the spectral weight function has a general dependence on the volume of the box and the physical width of the resonance in the resonance region. As we pointed out in our previous study [2], this opens up a possibility to extract the resonance parameters from the spectral weight functions obtained in Monte Carlo simulations. It is readily verified from Eq. (41) and Eq. (47) that, close to the energy of a resonance, both spectral weight functions satisfy the following functional form:

$$\frac{1}{W(E, L)} \simeq A(E) + \frac{B(E)\Gamma}{(E_\star - E)^2 + \Gamma^2/4} + \frac{C(E)}{\Delta E}, \quad (49)$$

where $A(E)$, $B(E)$ and $C(E)$ are smooth functions of the energy in the resonance region and they do not contain explicit volume dependence. The explicit volume dependence only comes from the term containing ΔE and the information about the resonance (i.e. E_\star and Γ) is encoded in the second term of the above equation. If one performs simulations on a series of volumes with the energies close to an underlying resonance and fits the spectral weight functions, it is in principle possible to extract the resonance parameters. Of course, the feasibility of this remains to be checked in realistic simulations.

Appendix A: Cubic harmonics for various irreducible representations

In this appendix, we list the cubic harmonics used in our calculation for various irreducible representations of the cubic group. We denote these cubic harmonics as $\mathcal{Y}_{l,i}^{(\Gamma)}(\mathbf{r})$ where Γ is the label for the irrep, l is the corresponding angular momentum label (for the rotational group) and $i = 1, \dots, \dim(\Gamma)$ denotes different basis functions of the irrep Γ . If Γ were one-dimensional, the

label i will be dropped. The functions $\mathcal{Y}_{l;i}^{(\Gamma)}(\mathbf{r})$ defined here are homogeneous functions of order l . We will also use the notation:

$$Y_{l;i}^{(\Gamma)}(\Omega_{\mathbf{r}}) = r^{-l} \cdot \mathcal{Y}_{l;i}^{(\Gamma)}(\mathbf{r}) \quad (\text{A1})$$

to designate the corresponding angular functions. It is easy to see that they are linear combinations of ordi-

nary spherical harmonics. Note that these functions are orthogonal to each other but some of them are *not* properly normalized. The table for these harmonics can be found in Ref. [5].

☞ **The A_1^+ channel:**

$$\left\{ \begin{array}{l} \mathcal{Y}_0^{(A_1^+)}(\mathbf{r}) = \mathcal{Y}_{00}(\mathbf{r}) , \\ \mathcal{Y}_4^{(A_1^+)}(\mathbf{r}) = \mathcal{Y}_{40} + \sqrt{\frac{5}{14}}(\mathcal{Y}_{4,4} + \mathcal{Y}_{4,-4}) \propto \left(x^4 + y^4 + z^4 - \frac{3}{5}r^4 \right) , \\ \mathcal{Y}_6^{(A_1^+)}(\mathbf{r}) = \left(x^2 y^2 z^2 + \frac{1}{22}r^2 \cdot \mathcal{Y}_4^{(A_1^+)}(\mathbf{r}) - \frac{1}{105}r^6 \right) , \\ \mathcal{Y}_8^{(A_1^+)}(\mathbf{r}) = \left(x^8 + y^8 + z^8 - \frac{28}{5}r^2 \cdot \mathcal{Y}_6^{(A_1^+)}(\mathbf{r}) - \frac{210}{143}r^4 \cdot \mathcal{Y}_4^{(A_1^+)}(\mathbf{r}) - \frac{1}{6}r^8 \right) , \\ \dots \end{array} \right. \quad (\text{A2})$$

☞ **The A_2^- channel:**

$$\left\{ \begin{array}{l} \mathcal{Y}_3^{(A_2^-)}(\mathbf{r}) = xyz , \\ \mathcal{Y}_7^{(A_2^-)}(\mathbf{r}) = xyz \left(x^4 + y^4 + z^4 - \frac{5}{11}r^4 \right) , \\ \dots \end{array} \right. \quad (\text{A3})$$

☞ **The E^+ channel:**

$$\left\{ \begin{array}{l} \mathcal{Y}_{2;1}^{(E^+)}(\mathbf{r}) = \left(z^2 - \frac{1}{2}(x^2 + y^2) \right) , \quad \mathcal{Y}_{2;2}^{(E^+)}(\mathbf{r}) = (x^2 - y^2) , \\ \mathcal{Y}_{4;1}^{(E^+)}(\mathbf{r}) = \left(z^4 - \frac{1}{2}(x^4 + y^4) - \frac{6}{7}r^2 \cdot \mathcal{Y}_{2;1}^{(E^+)}(\mathbf{r}) \right) , \quad \mathcal{Y}_{4;2}^{(E^+)}(\mathbf{r}) = \left(x^4 - y^4 - \frac{6}{7}r^2 \cdot \mathcal{Y}_{2;2}^{(E^+)}(\mathbf{r}) \right) , \\ \mathcal{Y}_{6;1}^{(E^+)}(\mathbf{r}) = \left(z^6 - \frac{1}{2}(x^6 + y^6) - \frac{11}{15}r^2 \cdot \mathcal{Y}_{4;1}^{(E^+)}(\mathbf{r}) - \frac{5}{7}r^4 \cdot \mathcal{Y}_{2;1}^{(E^+)}(\mathbf{r}) \right) , \\ \mathcal{Y}_{6;2}^{(E^+)}(\mathbf{r}) = \left(x^6 - y^6 - \frac{11}{15}r^2 \cdot \mathcal{Y}_{4;2}^{(E^+)}(\mathbf{r}) - \frac{5}{7}r^4 \cdot \mathcal{Y}_{2;2}^{(E^+)}(\mathbf{r}) \right) , \\ \dots \end{array} \right. \quad (\text{A4})$$

☞ **The T_1^- channel:**

$$\left\{ \begin{array}{l} \mathcal{Y}_{1;3}^{(T_1^-)}(\mathbf{r}) = \mathcal{Y}_{10}(\mathbf{r}) \propto z , \\ \mathcal{Y}_{3;3}^{(T_1^-)}(\mathbf{r}) = \mathcal{Y}_{30}(\mathbf{r}) \propto z \left(z^2 - \frac{3}{5}r^2 \right) , \\ \mathcal{Y}_{5;3}^{(T_1^-)}(\mathbf{r}) = z \left(z^4 - \frac{10}{9} \left(z^2 - \frac{3}{5}r^2 \right) r^2 - \frac{3}{7}r^4 \right) , \\ \mathcal{Y}_{5;3}^{(T_1^-)'}(\mathbf{r}) = z \left(x^4 + y^4 - \frac{3}{4}(x^2 + y^2)^2 \right) , \\ \dots \end{array} \right. \quad (\text{A5})$$

☞ The T_2^+ channel:

$$\left\{ \begin{array}{l} \mathcal{Y}_{2;3}^{(T_2^+)}(\mathbf{r}) = xy, \\ \mathcal{Y}_{4;3}^{(T_2^+)}(\mathbf{r}) = xy \left(z^2 - \frac{1}{7}r^2 \right), \\ \mathcal{Y}_{6;3}^{(T_2^+)}(\mathbf{r}) = xy \left(z^4 - \frac{6}{11}z^2r^2 + \frac{1}{33}r^4 \right), \\ \mathcal{Y}_{6;3}^{(T_2^+)' }(\mathbf{r}) = xy \left(x^4 + y^4 - \frac{5}{8}(x^2 + y^2)^2 \right), \\ \dots \end{array} \right. \quad (\text{A6})$$

Note that for the irrep T_1^- and T_2^+ , the basis functions is formed by 3 functions. Here we only list the ones that correspond to the z components. Other two sets can be obtained by cyclicly swapping the coordinates. It is also noted that at $l = 5$, we have two sets of basis (one of the basis function is denoted by a prime) since the irrep

T_1^- appears twice in the decomposition of $l = 5$. Similar situation occurs for irrep T_2^+ at $l = 6$. Since the function $G(\mathbf{r}; k)$ is cubic invariant, it is easy to verify that $\mathcal{G}_{l;i}^{(\Gamma)}$ defined in this Appendix indeed forms a basis for the corresponding representation Γ of the cubic group.

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 - [7] Here we adopt a convention for spherical Bessel functions as in Ref. [3].
 - [8] Note that this condition is somewhat different from the original condition imposed by Lüscher. We choose this condition because with this convention, the relation in Eq. (34) is in a simpler form.
 - [9] See for example pp. 555 of Ref. [6] for a derivation of this formula. According to Ref. [6], this formula was first obtained by Lüders in 1955.
 - [10] For convenience, a factor $(4\pi)/k^2$ is scaled out in the channel as opposed to $(4\pi)/k$ in the A_1^+ channel.